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Strong Stability Preserving properties of composition Runge-Kutta schemes*

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Abstract

In this paper Strong Stability Preserving (SSP) properties of Runge Kutta methods obtained by composing k different schemes with different step sizes are studied. The SSP coefficient of the composition method is obtained and an upper bound on this coefficient is given. Some examples are shown. In particular, it is proven that the optimal n^2-stage third order explicit Runge-Kutta methods obtained by D.I. Ketcheson [*SIAM J. Sci. Comput. 30(4), 2008*] are composition of first order SSP schemes.

Keywords Initial value problem Runge-Kutta composition method strong stability preservingSSP monotonicity radius of absolute monotonicity

Mathematics Subject Classification 65L05 65L06 65L20 65M20

1 Introduction

Given an initial value problem of the form

$$\begin{aligned} \frac{d}{dt}y(t) &= f(y(t))\,, \qquad t \geq t_0\,, \\ y(t_0) &= y_0\,, \end{aligned} \tag{1}$$

a common class of schemes to solve it are explicit Runge-Kutta (RK) methods. An s-stage explicit RK method is defined by a strictly lower triangular $s \times s$ matrix $A = (a_{ij})$ and a vector $b = (b_j) \in \mathbb{R}^s$. If y_n is the numerical approximation of the solution $y(t)$ at $t = t_n$, the numerical approximation of the solution at $t_{n+1} = t_n + h$, denoted by y_{n+1}, is obtained from

$$Y_i = y_n + h\sum_{j=1}^{s-1} a_{ij} f(Y_j)\,, \qquad 1 \leq i \leq s\,, \tag{2}$$

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(Y_i)\,, \tag{3}$$

*This is a pre-print of an article published in Journal of Scientific Computing. The final authenticated version is available online at: https://doi.org/10.1007/s10915-019-00956-9 where the internal stage Y_i approximates $y(t_n + c_i h)$, and, as usual, $c_i = \sum_{j=1}^{s-1} a_{ij}$.

Composition methods have been widely studied in the literature (see, e.g., [1, 11, 12, 17, 18] and the references therein). The basic idea is to consider k ordered Runge-Kutta methods and, from an initial value y_0, compute a numerical approximation y^1 using the first scheme with step size h_1; next, from y^1 the process is repeated to compute a numerical approximation y^2 using the second scheme with step size h_2. This process continues until a numerical solution y^k is computed with the last h_k-step size Runge-Kutta method. The composition of these schemes is considered as a single method that is used to compute, from y_0, a numerical solution $y_1 = y^k$ with step size $h = h_1 + \cdots + h_k$. Composition schemes are aimed at increasing the convergence order while relevant properties of the method are preserved. For this purpose, properties of the composition method must be studied in terms of the ones of the Runge-Kutta schemes involved and the step sizes used.

Different kinds of composition methods and different properties have been studied in the literature. For example, in [11, Section III.1.3] (see too [12, Section II.12]), composition of two different Runge-Kutta methods with the same step size is considered and order properties of the new scheme are derived in terms of those of the original two methods. In [11, Section II.4], the composition of a basic one-step method (and eventually, its adjoint method) with k different step sizes is studied and order conditions to increase the order of the basic one-step method are given; in this way, high order symplectic and symmetric methods are obtained by composition of low order schemes. In [17, 18], composition of low order Runge-Kutta methods with different step sizes to improve stability for stiff problems is analyzed.

In this paper we consider the most general case where different Runge-Kutta methods are composed with different step sizes. Thus, given k s_i-stage Runge-Kutta methods (A_i, b_i^t) satisfying the first order conditions $b_i^t e_{s_i} = 1$, where $e_{s_i} = (1, \dots, 1)^t \in \mathbb{R}^{s_i}$, $i = 1, \dots, k$, we consider their composition with step sizes $d_i h$, $i = 1, \dots, k$, such that $d_1 + \cdots + d_k = 1$, with $d_i > 0$, $i = 1, \dots, k$. The composition method is an s-stage Runge-Kutta method, with $s = s_1 + \cdots + s_k$, whose Butcher matrix is of the form

$$
\begin{array}{c|ccccc}
d_1 c_1 & d_1 A_1 & 0 & \cdots & \cdots & 0 \\
d_1 e_{s_2} + d_2 c_2 & d_1 e_{s_2} b_1^t & d_2 A_2 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \ddots & 0 \\
\left(\sum_{i=1}^{k-2} d_i\right) e_{s_{k-1}} + d_{k-1} c_{k-1} & d_1 e_{s_{k-1}} b_1^t & d_2 e_{s_{k-1}} b_2^t & \cdots & d_{k-1} A_{k-1} & 0 \\
\left(\sum_{i=1}^{k-1} d_i\right) e_{s_k} + d_k c_k & d_1 e_{s_k} b_1^t & d_2 e_{s_k} b_2^t & \cdots & d_{k-1} e_{s_k} b_{k-1}^t & d_k A_k \\
\hline
(A, b^t) & d_1 b_1^t & d_2 b_2^t & \cdots & d_{k-1} b_{k-1}^t & d_k b_k^t
\end{array} \tag{4}
$$

Observe that, for the composition method (A, b^t), the first blocks in vector b^t, namely $d_i b_i^t$, $i = 1, \dots, k-1$, are the same as the ones in the last row of A; in this way, the structure of the Butcher tableau allows us to detect easily whether or not a Runge-Kutta method is a composition scheme. On the other hand, it is well known that the stability function of a composition method is the product of the stability functions of the schemes involved in the composition [17]; thus the stability function can also be used to analyze if a given method is a composition one.

For differential systems (1) with a large number of equations N, the high dimension of the problem may compromise the computer memory capacity and thus it is convenient to take into account the memory usage of the scheme (see, e.g., [20] and the references therein). From this point of view, composition Runge-Kutta methods may be competitive with general Runge-Kutta methods with the same number of stages. A plain implementation of an s-stage Runge-Kutta method requires $s + 1$ memory registers of length N. However, for a general composition method (4), the number of memory registers required to implement the method can be reduced to $\max_{i=1,\dots,k}\{s_i\}+1$ registers, and this diminution is even better if all the schemes involved in the composition are low-storage methods.

As it has been pointed out above, one of the goals of constructing composition schemes is to increase the order while preserving important properties of the schemes involved. In this paper, we deal with Strong Stability Preserving (SSP) Runge-Kutta schemes.

SSP methods were introduced in the context of hyperbolic problems to ensure numerical monotonicity for the Total Variation seminorm [9, 28, 29]; in this context, SSP methods are also known as Total Variation Diminishing (TVD) methods. Numerical contractivity, closely related to numerical monotonicity, has also been studied in the seminal paper by Kraaijevanger [24]. Stepsize restrictions for numerical monotonicity or contractivity are given as the product of two coefficients, one that depends on the problem and the other one that depends on the numerical method used. Depending on the context, the coefficient associated to the scheme is known as SSP coefficient, CFL coefficient, Kraaijevanger coefficient or radius of absolute monotonicity (see, e.g., [6], [8, 27], [16], [24], respectively).

Different issues on SSP Runge-Kutta methods have been deeply studied in the literature. In [4, 14], the relationship between the SSP coefficient [28, 29] and the radius of absolute monotonicity [24] is established (see also [3, 13]). For a given order and number of stages, explicit and implicit optimal SSP schemes have been studied in [26, 27, 33, 34] and [5, 21], respectively; besides, optimal SSP methods can be constructed with the code RKOpt [22]. A more general framework for analyzing SSP methods is introduced in [32]; this framework can be applied to different kinds of methods like additive Runge-Kutta methods [15], General Linear Methods, Linear Multistep methods or multistep-multistage methods. With regard to implementation issues, low-storage SSP methods have been analyzed in [19, 26]. For linear problems, monotonicity properties of the Runge-Kutta scheme are obtained from the stability function of the method [30, 31]. Thus, the study for explicit and implicit schemes is reduced to the analysis of absolute monotonicity for polynomials [23] and rational functions [10], respectively. See too [7] and the references therein.

The aim of this paper is to study SSP properties of composition Runge-Kutta methods. Our goal is to increase the order and, at the same time, preserve or improve SSP properties of the involved schemes. The main results of the paper are the following ones:

- We obtain the SSP coefficient of the composition method in terms of the SSP coefficients of the schemes involved. Furthermore, an upper bound for the SSP coefficient of the composition method is also given. These results, valid for explicit and implicit Runge-Kutta methods, are given in Proposition 1.

- We obtain a fourth order explicit SSP Runge-Kutta composition method.

- We prove in Proposition 3 that optimal n^2-stage third order explicit SSP Runge-Kutta schemes introduced in [19] are the composition of first order SSP Runge-Kutta methods. Then we obtain the SSP coefficient of this composition method from Proposition 1.

Besides, in Proposition 2 we give the simplified order conditions needed to obtain a third order composition method starting from first order schemes.

The rest of the paper is organized as follows. In Section 2 we give a brief introduction to SSP Runge-Kutta methods. The main results of the paper are given in Section 3. The order conditions needed to obtain a third order composition method are given in Section 4; they are needed for the examples shown later in the paper. In this section we also obtain a fourth order explicit SSP composition method. Section 5 is devoted to examples of explicit and implicit composition Runge-Kutta methods; among them, we study the optimal n^2-stage third order explicit SSP Runge-Kutta schemes obtained in [19] (see too [7, p. 85]). The paper ends with some conclusions. In Section 7 we give the proofs of the results in the paper together with two auxiliary lemma. We have collected them in a separate section in order not to interrupt the reading of the paper.

2 Strong Stability Preserving Runge-Kutta methods

In this section we briefly review some known concepts on SSP methods that will be used throughout this paper. These methods are relevant for dissipative problems (1), that is, problems such that the exact solution satisfies a monotonicity property of the form

$$\|y(t)\| \leq \|y(t_0)\|\,, \qquad \text{for all } \ t \geq t_0\,, \tag{5}$$

where $\|\cdot\| : \mathbb{R}^N \to \mathbb{R}$ denotes a convex functional (e.g., a norm or a semi-norm). A sufficient condition for (5) is monotonicity under explicit Euler steps

$$\|\, y + \, h\, f(y)\,\| \leq \|\, y\,\|\,, \qquad \text{for } h \leq \Delta t_{EE}. \tag{6}$$

for all $y \in \mathbb{R}^N$ and a fixed $\Delta t_{EE} > 0$ (see, e.g., [24, p. 501] or [15, p. 1-2] for details).

As usually, $c_i \geq 0.$ As $Y_i \approx y(t_n + c_i h)$, taking into account (5), it makes sense to impose numerical monotonicity not only for the numerical solution but also for the internal stages, that is,

$$\|Y_i\| \leq \|y_n\|\,, \qquad i = 1\,\ldots, s\,, \qquad\qquad \|y_{n+1}\| \leq \|y_n\|\,, \tag{7}$$

for all $n \geq 0$, probably under a stepsize restriction $h \leq \Delta t_{_{MAX}}$. The seminal papers by Spijker [30, 31, 32] and Kraaijevanger [23, 24] on numerical contractivity issues for Runge-Kutta schemes, settle a theoretical framework that is valid not only for contractivity but also for monotonicity.

With a different terminology and notation, the numerical preservation of monotonicity has also been investigated in the context of hyperbolic systems of conservation laws. In this setting, for different reasons, it is critical to deal with Total Variation Diminishing (TVD) schemes, and in the pioneering papers [28, 29], monotonicity issues for the Total Variation semi-norm are analyzed. In these references, high order methods satisfying (7) when the explicit Euler discretization of (1) satisfies (6) are studied. In this context, these methods are known as SSP methods.

The idea in [24, 28, 29] is to construct high order schemes by means of convex combinations of explicit Euler steps. Thus, Runge-Kutta methods (2-3), that in compact form can be written as

$$Y = e_N \otimes y_n + (\mathbb{A} \otimes I_N) F(Y)\,,$$

where $\otimes$ denotes the Kronecker product, $Y = (Y_1, \ldots, Y_s, y_{n+1})^t \in \mathbb{R}^{(s+1)N}$, $F(Y) = (f(Y_1), \ldots, f(Y_s), 0)^t \in \mathbb{R}^{(s+1)N}$, and

$$\mathbb{A} = \begin{pmatrix} A & 0 \\ b^t & 0 \end{pmatrix}\,, \tag{8}$$

are expressed as

$$Y = \alpha_r \otimes y_n + (\Lambda_r \otimes I_N) \left(Y + \frac{h}{r} F(Y) \right)\,, \tag{9}$$

where $r \in \mathbb{R}$ and

$$\alpha_r = (I + r\mathbb{A})^{-1} e_{s+1}\,, \qquad \Lambda_r = r(I + r\mathbb{A})^{-1}\mathbb{A}\,. \tag{10}$$

If $\alpha_r \geq 0$ and $\Lambda_r \geq 0$, where the inequalities should be understood component-wise, then the right hand side of (9) is a convex combination of y_n and explicit Euler steps. The radius of absolute monotonicity, also known as Kraaijevanger's coefficient or SSP coefficient, is denoted and defined by

$$R(\mathbb{A}) = \sup \left\{ r \,|\, r = 0 \text{ or } r > 0, (I + r\mathbb{A})^{-1} \text{ exits, and } \alpha_r \geq 0, \Lambda_r \geq 0 \right\}\,. \tag{11}$$

Blockwise, conditions in (11) can be written as

$$(I + rA)^{-1}A \geq 0\,, \quad (I + rA)^{-1}e_s \geq 0\,, \quad b^t(I + rA)^{-1} \geq 0\,, \quad 1 - rb^t(I + rA)^{-1}e_s \geq 0\,. \tag{12}$$

If the explicit Euler method satisfies condition (6), then from (9), numerical monotonicity (7) can be proven under the step size restriction

$$h \leq R(\mathbb{A})\, \Delta t_{EE}\,.$$

It is well known that, for an irreducible SSP Runge-Kutta method (A, b^t), the coefficients must satisfy $a_{ij} \geq 0$, $b_j > 0$ (see [24, Theorem 4.2]). This sign condition implies an order barrier $p \leq 4$ and $p \leq 6$ for explicit and implicit SSP methods, respectively [24, Corollary 8.7].

Expression (9) is a particular case of Shu-Osher representations of a Runge-Kutta method (see, e.g., [14, Section 2]). Given a Runge-Kutta method with Butcher matrix $\mathbb{A}$, a representation is given in terms of two matrices (Λ, Γ) such that the matrix $I - \Lambda$ is invertible and $\mathbb{A} = (I - \Lambda)^{-1}\Gamma$; then the numerical approximation of the Runge-Kutta scheme is written as

$$Y = \alpha \otimes y_n + (\Lambda \otimes I_N)Y + h(\Gamma \otimes I_N)F(Y)\,, \tag{13}$$

where $\alpha = (I - \Lambda)e$. We can consider $\alpha = (1, 0, \ldots, 0)^t$ for explicit methods as $Y_1 = y_n$. Adding and subtracting the term $r(\Gamma \otimes I_N)Y$, equation (13) can also be written as

$$Y = \alpha \otimes y_n + ((\Lambda - r\,\Gamma) \otimes I_N)\,Y + r(\Gamma \otimes I_N)\left(Y + \frac{h}{r}F(Y)\right)\,. \tag{14}$$

If

$$\Lambda \geq 0\,, \quad \Gamma \geq 0\,, \quad \alpha \geq 0\,, \quad \Lambda - r\,\Gamma \geq 0\,, \tag{15}$$

then the right hand side of equation (14) is a convex combination of y_n, the internal stages and forward Euler steps. For $r = \mathcal{R}(\mathbb{A})$, it can be proven [14, Proposition 2.7] that there exist Shu-Osher representations (Λ, Γ) of $\mathbb{A}$ such that inequalities (15) hold. Observe that the largest value r in (15) that satisfies $\Lambda - r\,\Gamma \geq 0$ is given by $r = \min_{ij}\{\lambda_{ij}/\gamma_{ij}\}$, that agrees with the SSP coefficient of a Runge-Kutta method defined in the context of TVD schemes (see, e.g., [28]; see also [7] and the references therein). In other words, these representations are optimal. For example, α_r and Λ_r in (10), together with $\Gamma_r := \Lambda_r/r$ give an optimal representation. Observe that, in this case, $\Lambda_r - r\Gamma_r = 0$ and thus (14) is reduced to (9).

Optimal explicit SSP Runge-Kutta methods for a given order p and a number of stages s, denoted by $SSP(s, p)$, have been studied in the literature. In [24, Section 9], optimal $SSP(s, 1)$, $SSP(s, 2)$, $SSP(3, 3)$ and $SSP(4, 3)$ are given. Optimal $SSP(n^2, 3)$ schemes were found in [19] in the context of low-storage methods. Numerically optimal SSP methods, in the sense that the schemes have been constructed with numerical optimization techniques but no formal proof of optimality has been done, are also given in the literature [26, 33, 34]; furthermore, they can also be constructed with the code RKOpt [22]. With regard to implicit methods, optimal SSP SDIRK schemes were studied in [5] and general implicit SSP methods can be reviewed in [21] (see too [7, Chapter 7]).

For explicit Runge-Kutta methods, an upper bound of the SSP coefficient can be given in terms of the Butcher coefficients of the scheme [27, Lemma 3.2],

$$R(\mathbb{A}) \leq \frac{1}{\max\{a_{ij}, b_j\}}\,. \tag{16}$$

This is a bound of practical relevance because it is easy to compute and, reversely, if we fix $R(\mathbb{A})$, (16) trivially implies an upper bound of the coefficients of the Runge-Kutta method

$$\max\{a_{ij}, b_j\} \leq \frac{1}{R(\mathbb{A})}\,. \tag{17}$$

It can be checked that for optimal methods $SSP(s,1)$, $SSP(s,2)$, $SSP(3,3)$, $SSP(4,3)$ in [24], and $SSP(s,3)$, $s = 5,\dots,8$, in [26], the non zero entries in first rows of matrix A are equal to $1/R(\mathbb{A})$. This is also the case for the optimal scheme $SSP(10,4)$ given in [19]. However, the optimal $SSP(5,4)$ method does not have this property [24, 33].

For linear problems, SSP properties can be obtained from the stability function of the Runge-Kutta method, defined as

$$\phi(z) = 1 + zb^t(I - zA)^{-1}e_s\,.$$

For explicit Runge-Kutta methods, optimal stability functions were obtained in [23] whereas results for implicit schemes can be seen in [10]. For first and second order s-stage optimal Runge-Kutta methods, the SSP coefficient for linear and nonlinear problems is the same; this is also the case for some third order optimal or numerically optimal SSP schemes [6, Table 3].

For a detailed study on numerical monotonicity and SSP methods, see the references in Section 1.

3 SSP coefficient of composition methods

In this section we give some results on the SSP coefficient of a Runge-Kutta method that is the composition of k SSP Runge-Kutta schemes. For simplicity, we have written down the proof of each result in section 7.

Proposition 1. *Consider a Runge-Kutta method $\mathbb{A}$ that is the composition of k first order SSP schemes $\mathbb{A}_i$ with step sizes $d_i h$, such that $d_i > 0$, $i = 1,\dots,k$, and $d_1 + \cdots + d_k = 1$. Then, the SSP coefficient $R(\mathbb{A})$ for the composition method is*

$$R(\mathbb{A}) = \min_{i=1,\dots,k} \left\{ \frac{R(\mathbb{A}_i)}{d_i} \right\}\,. \tag{18}$$

Furthermore, if we define $\mathcal{I}_k = \{i \in \{1,\dots,k\} \mid R(\mathbb{A}_i) < \infty\}$ and we assume that $\mathcal{I}_k \neq \emptyset$, then

$$R(\mathbb{A}) \leq \frac{\displaystyle\sum_{i\in\mathcal{I}_k} R(\mathbb{A}_i)}{\displaystyle\sum_{i\in\mathcal{I}_k} d_i}\,, \tag{19}$$

and the maximum value for $R(\mathbb{A}) = \sum_{i\in\mathcal{I}_k} R(\mathbb{A}_i)/\sum_{i\in\mathcal{I}_k} d_i$ *is obtained if and only if*

$$d_i = \frac{\sum_{j\in\mathcal{I}_k} d_j}{\sum_{j\in\mathcal{I}_k} R(\mathbb{A}_j)} R(\mathbb{A}_i)\,, \quad i \in \mathcal{I}_k\,. \tag{20}$$

In particular, if $R(\mathbb{A}_i) < \infty$, for $i = 1, \dots, k$, then

$$R(\mathbb{A}) \leq R(\mathbb{A}_1) + \cdots + R(\mathbb{A}_k)\,,$$

and the maximum value $R(\mathbb{A}) = R(\mathbb{A}_1) + \cdots + R(\mathbb{A}_k)$ is obtained if and only if

$$d_i = \frac{R(\mathbb{A}_i)}{R(\mathbb{A}_1) + \cdots + R(\mathbb{A}_k)}.$$

Thus, given k SSP Runge-Kutta methods, it is always possible to construct a new SSP scheme with larger SSP coefficient and more stages. However, in order to increase the order of the composition scheme, the coefficients d_i must satisfy some order conditions (see section 4).

Remark 1.

1. Observe that, as expected, the SSP coefficient of the composition method does not depend on the position of each $\mathbb{A}_i$ method in the composition process.

2. Recall that Proposition 1 is valid for both implicit and explicit Runge-Kutta methods. □

As we have pointed out above, one of the goals of constructing composition schemes is to increase the order at the same time that important properties are preserved. Next, we study order conditions of composition methods.

4 Order conditions of composition methods

Given a Runge-Kutta method (A, b^t), the set of order conditions to achieve third order is well known:

$$b^t e = 1\,, \qquad b^t c = \frac{1}{2}\,, \qquad b^t c^2 = \frac{1}{3}\,, \qquad b^t A c = \frac{1}{6}\,. \tag{21}$$

However, in the analysis or construction of composition methods with large or arbitrary number of stages, the determination of the order with these standard conditions (21) may become a laborious task. The problem can be simplified if we consider the method as a composition scheme [17, 18]. In this section we give the second and third order conditions for the composition method in terms of the order conditions of the involved schemes and the step-length ratios d_i, $i = 1, \dots, k$. We will use them for the examples given in section 3.

Proposition 2. *We consider a Runge-Kutta method* (A, b^t) *that is the composition of* k *first order Runge-Kutta methods* (A_i, b_i^t)*, with step sizes* $d_i h$*, such that* $d_i > 0$*,* $i = 1, \dots, k$*, and* $d_1 + \cdots + d_k = 1$*, with* $d_i > 0$*,* $i = 1, \dots, k$*, then*

1. *The second order condition $b^t c = 1/2$ for the composition method is equivalent to*

$$\sum_{i=1}^{k} d_i^2 (b_i^t c_i - \tfrac{1}{2}) = 0\,. \tag{22}$$

2. *The third order condition $b^t c^2 = 1/3$ for the composition method is given by*

$$\sum_{i=1}^{k} d_i^3 (b_i^t c_i^2 - \tfrac{1}{3}) + 2 \sum_{i=2}^{k} \left(\sum_{j=1}^{i-1} d_j \right) d_i^2 (b_i^t c_i - \tfrac{1}{2}) = 0\,. \tag{23}$$

   If the second order condition (22) *holds, then the third order condition $b^t Ac = 1/6$ is equivalent to*

$$\sum_{i=1}^{k} d_i^3 \left((b_i^t A_i c_i - \tfrac{1}{6}) - (b_i^t c_i - \tfrac{1}{2}) \right) = 0\,. \tag{24}$$

The proof of this result is given in section 7.

The order conditions (22)-(24) are extremely useful to obtain the order of a given composition method or to construct second and third order composition schemes. Besides, they can also be used to obtain necessary conditions on the methods used in the composition or, equivalently, to prove that the composition of some schemes never achieves a given order. For example, from (22), we conclude that the expressions $b_i^t c_i - \frac{1}{2}$, $i = 1, \ldots, s$, must have different signs; in particular, second order cannot be achieved by concatenating the same first order scheme. In a similar way, from (23), third order cannot be achieved by the composition of the same second order method. Another straightforward conclusion obtained from (22) is that a second order composition method cannot be obtained from the composition of a first and a second order method.

Remark 2.

1. Observe that, in equations (22) and (24), the arrangement of the different schemes in the composition method is not relevant to fulfill them. This result is not surprising because $b^t c = 1/2$ and $b^t Ac = 1/6$ are the order conditions for linear problems, and they are included in the stability function of a method. It is well known that the stability function of a composition method is the product of the stability functions of the schemes involved in the composition [17] and thus, the order of the factors is irrelevant. However, the arrangement of the different schemes is relevant for the non linear condition (23).

2. The composition of different one-step methods of order p is considered in [18]; in particular, the order conditions needed to construct a composition method with order $p + 1$ are given in [18, Theorem 1]. However, in Proposition 2 we give the order conditions needed to obtain a third order composition method starting from first order schemes.

□

In Proposition 1 we have shown that the composition of SSP methods is also an SSP scheme. Consequently, the SSP order barriers, namely $p \leq 4$ and $p \leq 6$ for explicit and implicit methods, respectively, are also valid for the composition of SSP methods. We wonder whether there exist fourth order SSP explicit Runge-Kutta schemes obtained by composing lower order explicit SSP methods. We answer this question in the next subsection.

4.1 Fourth order SSP explicit composition Runge-Kutta methods

In this section we try to construct a fourth order method by composing two third order schemes, denoted by (A_1, b_1) and (A_2, b_2), with positive step-length ratios d_1 and d_2, such that $d_1 + d_2 = 1$. The fourth order conditions for the composition method, that can be obtained from [18, Theorem 1], are

(25)

$$d_1^4 \left(b_1^t A_1^2 c_1 - \frac{1}{24} \right) + d_2^4 \left(b_2^t A_2^2 c_2 - \frac{1}{24} \right) = 0 , \qquad d_1^4 \left(b_1^t A_1 c_1^2 - \frac{1}{12} \right) + d_2^4 \left(b_2^t A_2 c_2^2 - \frac{1}{12} \right) = 0 ,$$

$$d_1^4 \left(b_1^t c_1^3 - \frac{1}{4} \right) + d_2^4 \left(b_2^t c_2^3 - \frac{1}{4} \right) = 0 , \qquad d_1^4 \left(b_1^t (A_1 c_1 \cdot c_1) - \frac{1}{8} \right) + d_2^4 \left(b_2^t (A_2 c_2 \cdot c_2) - \frac{1}{8} \right) = 0 .$$

If we consider (25) as a linear system $Md = 0$, with unknowns $d = (d_1^4, d_1^4)$ and $M = (m_{ij})$, we obtain that (25) has a positive solution if and only if $K m_{i1} = m_{i2}$, $i = 1, \ldots, 4$, with $K < 0$, that is,

$$\begin{aligned} &K \left(b_1^t A_1^2 c_1 - \frac{1}{24} \right) = b_2^t A_2^2 c_2 - \frac{1}{24} , \qquad && K \left(b_1^t A_1 c_1^2 - \frac{1}{12} \right) = b_2^t A_2 c_2^2 - \frac{1}{12} , \\ &K \left(b_1^t c_1^3 - \frac{1}{4} \right) = b_2^t c_2^3 - \frac{1}{4} , && K \left(b_1^t (A_1 c_1 \cdot c_1) - \frac{1}{8} \right) = b_2^t (A_2 c_2 \cdot c_2) - \frac{1}{8} . \end{aligned} \tag{26}$$

In this case, equations (25) are reduced to $d_1^4 + K d_2^4 = 0$.

Observe that conditions (26) can be considered as four *pseudo* order conditions, easier to check than standard fourth order Runge-Kutta equations. We have considered these conditions in the numerical optimization process to get the 21 unknowns, namely, the coefficients of both methods (A_1, b_1^t) and (A_2, b_2^t), and the parameter K, that give the largest value of the SSP coefficient of the composite method $R(\mathbb{A})$. More precisely, the following optimization problem has been solved:

Maximize $R(\mathbb{A})$ subject to:

(27)

Third order conditions (21) for methods $(A_i, b_i^t)\,, i = 1, 2.$
Positivity of the non-zero coefficients of schemes $(A_i, b_i^t)\,, i = 1, 2.$
$K m_{i1} = m_{i2},\ i = 1, \ldots, 4$, with $K < 0\,.$

Once that K is known, from $d_1 + d_2 = 1$ and $d_1^4 + K d_2^4 = 0$, the step-length ratios d_1 and d_2 can be obtained. In this way, we obtain an 8-stage fourth order SSP Runge-Kutta method (A, b^t) with maximal SSP coefficient $R(\mathbb{A}) = 0.8561887$, that is the composition of the following 4-stage third order SSP Runge-Kutta methods (A_1, b_1^t) and (A_2, b_2^t)

0	0	0	0	0
1.355799533961411	1.355799533961411	0	0	0
0.382966116123274	0.130435927623664	0.252530188499610	0	0
0.456559352213873	0.061507046874709	0.029346849161985	0.365705456177179	0
(A_1, b_1^t)	0.064411678388945	0.088196417893538	0.087798298497448	0.759593605220069

0	0	0	0	0
0.325452697522574	0.325452697522574	0	0	0
0.517030163135817	0.077328101144592	0.439702061991226	0	0
0.821413740789189	0.026827996375588	0.152548997366219	0.642036747047382	0
(A_2, b_2^t)	0.131599472101293	0.346443702425774	0.136319923552512	0.385636901920421

with step-length ratios $d_1 = 0.3688662$ and $d_2 = 0.6311338$. The SSP coefficients of each method are $R(\mathbb{A}_1) = 0.3160628$ and $R(\mathbb{A}_2) = 0.5403697$. Besides, in agreement with formula (18), the SSP coefficient of the composition method (A, b^t) is $R(\mathbb{A}) = 0.8561887$; observe that in this case, $R(\mathbb{A}_1)/d_1 = R(\mathbb{A}_2)/d_2$ and $R(\mathbb{A}) = R(\mathbb{A}_1) + R(\mathbb{A}_2)$. For (A_1, b_1^t) and (A_2, b_2^t) the *pseudo* order conditions (26) are satisfied for $K = -0.1166781$.

We remark that this example is intended to show that fourth order composition methods exist. A detailed study on the largest SSP coefficient for composition schemes is out of the scope of this paper.

5 Examples

In this section we give some examples of composition schemes.

Example 1. We consider the composition of s implicit midpoint rule methods, (A_i, b_i^t), where $a_{11}^{(i)} = 1/2$, $b_1^{(i)} = 1$, with $d_i = 1/s$, $i = 1, \dots, s$. The Butcher tableau for the composition method $\mathbb{A}$ is

$$\begin{array}{c|cccc} \frac{1}{2s} & \frac{1}{2s} & 0 & \dots & 0 \\ \frac{3}{2s} & \frac{1}{s} & \frac{1}{2s} & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 0 \\ \frac{2s-1}{2s} & \frac{1}{s} & \frac{1}{s} & \dots & \frac{1}{2s} \\ \hline & \frac{1}{s} & \frac{1}{s} & \dots & \frac{1}{s} \end{array} \tag{28}$$

For each scheme, $R(\mathbb{A}_i) = 2$, $i = 1, \dots, s$. Then Proposition 1 gives us $R(\mathbb{A}) = 2s$. Furthermore, as implicit midpoint rule is a second order scheme, the second order condition (22) for the composition method is satisfied. Schemes (28) are well known in the literature: for $s = 1, 2$, they are the optimal SSP second order s-stage implicit DIRK schemes, and for $s \geq 3$ they are the numerically optimal ones found in [5] (see too [7, p. 95]). □

Example 2. We consider the composition of the following first, second and first order, respectively, implicit schemes

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{2}{3} & \frac{1}{3} & \frac{1}{3} \\ \hline (A_1, b_1^t) & \frac{1}{3} & \frac{2}{3} \end{array}, \qquad \begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline (A_2, b_2^t) & 1 \end{array}, \qquad \begin{array}{c|c} 1 & 1 \\ \hline (A_3, b_3^t) & 1 \end{array},$$

with step-length ratios $d_1 = 1/2$, $d_2 = 1/3$ and $d_3 = 1/6$. Their SSP coefficients are $R(\mathbb{A}_1) = 3$, $R(\mathbb{A}_2) = 2$, $R(\mathbb{A}_3) = \infty$. According to (18) in Proposition 1, we get $R(\mathbb{A}) = 6$. Observe that the maximum value in (19), namely $R(\mathbb{A}) = 6$, is achieved. In this case, the second order condition (22) for the composition method is

$$-\frac{1}{18} d_1^2 + \frac{1}{2} d_3^2 = 0 \,,$$

that is satisfied for the above values of d_1 and d_3. Thus, the 4-stage second order implicit Runge-Kutta composition method

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{6} & \frac{1}{6} & 0 & 0 \\ \frac{2}{3} & \frac{1}{6} & \frac{1}{3} & \frac{1}{6} & 0 \\ 1 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \\ \hline (A, b^t) & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}$$

with $R(\mathbb{A})=6$ is obtained. This composition method has been considered in [25]. Other similar schemes in the literature can also be obtained as composition methods. For example, we may consider the composition of these three first order schemes

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{8}{9} & \frac{4}{9} & \frac{4}{9} \\ \hline (A_1, b_1^t) & \frac{4}{9} & \frac{5}{9} \end{array}, \qquad \begin{array}{c|c} \frac{2}{7} & \frac{2}{7} \\ \hline (A_2, b_2^t) & 1 \end{array}, \qquad \begin{array}{c|c} 1 & 1 \\ \hline (A_3, b_3^t) & 1 \end{array},$$

with step-length ratios $d_1 = 3/5$, $d_2 = 7/30$ and $d_3 = 1/6$. Their SSP coefficients are $R(\mathbb{A}_1) = 9/4$, $R(\mathbb{A}_2) = 7/5$, $R(\mathbb{A}_3) = \infty$. Now, from (18) in Proposition 1, we get $R(\mathbb{A}) = 15/4$. In this case, the maximum value in (19), namely 4.38, is not achieved. The step-length ratios satisfy the second order condition (22) for the composition method

$$-\frac{1}{162}\, d_1^2 - \frac{3}{14}\, d_2^2 + \frac{1}{2}\, d_3^2 = 0\,.$$

Consequently, the 4-stage composition method (A, b^t) below, also considered in [2], is a second order scheme with $R(\mathbb{A}) = 15/4$.

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{8}{15} & \frac{4}{15} & \frac{4}{15} & 0 & 0 \\ \frac{2}{3} & \frac{4}{15} & \frac{1}{3} & \frac{1}{15} & 0 \\ 1 & \frac{4}{15} & \frac{1}{3} & \frac{7}{30} & \frac{1}{6} \\ \hline (A, b^t) & \frac{4}{15} & \frac{1}{3} & \frac{7}{30} & \frac{1}{6} \end{array}$$

□

Example 3. We consider the composition of the following first-order explicit Runge-Kutta methods

(29)
$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 2 & 1 & 1 & 0 \\ \hline (A_1, b_1^t) & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{array}, \qquad \begin{array}{c|c} 0 & 0 \\ \hline (A_2, b_2^t) & 1 \end{array},$$

with step sizes $d_1 h$ and $d_2 h$, with $d_1 + d_2 = 1$, $d_1, d_2 > 0$. For these methods the coefficients involved in the second and third order conditions (22-24) for the composition method are

$$b_1^t c_1 - \tfrac{1}{2} = \tfrac{1}{2}\,, \quad b_2^t c_2 - \tfrac{1}{2} = -\tfrac{1}{2}\,, \quad b_1^t c_1^2 - \tfrac{1}{3} = \tfrac{4}{3}\,, \quad b_2^t c_2^2 - \tfrac{1}{3} = -\tfrac{1}{3}\,, \quad b_1^t \mathcal{A}_1 c_1 - \tfrac{1}{6} = \tfrac{1}{6}\,, \quad b_2^t \mathcal{A}_2 c_2 - \tfrac{1}{6} = -\tfrac{1}{6}\,.$$

With these coefficients the second order condition (22) is reduced to $d_1^2 - d_2^2 = 0$. Then, together with equation $d_1 + d_2 = 1$, we obtain $d_1 = d_2 = 1/2$. Third order conditions (23)-(24) are satisfied with these step-length ratios. Consequently, the composition of methods (29), with step sizes $h/2$, gives us the third order method with Butcher tableau

(30)
$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & 0 \\ \hline & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{2} \end{array}$$

Furthermore, the SSP coefficients of the schemes (A_1, b_1^t) and (A_2, b_2^t) are $R(\mathbb{A}_1) = R(\mathbb{A}_2) = 1$, and thus, from (18), we obtain that the SSP coefficient for (30) is $R(\mathbb{A}) = 2$. Recall that method (30) is the optimal 4-stage third order SSP method [24, Theorem 9.5].

If we change the composition order of methods (29), that is, we advance first with the 1-stage method and secondly with the 3-stage one, then the second order condition (22) is reduced again to $d_1^2 - d_2^2 = 0$ and we get $d_1 = d_2 = 1/2$. However, the third order condition (23), now

$$-\frac{1}{3}\,d_1^3 + \frac{4}{3}\,d_2^3 + d_1 d_2^2 = 0\,,$$

is not satisfied and the composition method cannot achieve third order. □

In the next subsection we study optimal n^2- stage SSP explicit Runge-Kutta methods.

5.1 Optimal n^2- stage SSP explicit Runge-Kutta methods

Optimal n^2- stage SSP explicit Runge-Kutta methods were found in [19]. In this section we study the structure of these schemes for $n \geq 3$. We begin by proving a technical lemma whose proof is given in section 7.

Lemma 1. *Consider an s-stage explicit Runge-Kutta method of the form*

$$\text{(31)} \qquad \begin{array}{c|cccc} 0 & 0 & 0 & \cdots & 0 \\ \alpha & \alpha & 0 & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ (s-1)\alpha & \alpha & \cdots & \alpha & 0 \\ \hline & \beta & \beta & \cdots & \beta \end{array}$$

with $\alpha > \beta > 0$. Then:

1. *The SSP coefficient of the method is $R(\mathbb{A}) = 1/\alpha$.*
2. *The left hand side of the first, second and third order conditions* (21) *are*

(32)
$$b^t e = s\,\beta\,, \qquad b^t c = \frac{1}{2}\alpha\beta(s-1)s\,, \qquad b^t c^2 = \frac{1}{6}\alpha^2\beta(s-1)s(2s-1)\,, \qquad b^t A c = \frac{1}{6}\alpha^2\beta(s-2)(s-1)s\,.$$

Some well known optimal SSP methods are of the form (31).

Example 4.

1. The first order s-stage optimal SSP methods [24, Theorem 9.2]

$$\text{(33)} \qquad \begin{array}{c|cccc} 0 & 0 & 0 & \cdots & 0 \\ \frac{1}{s} & \frac{1}{s} & 0 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \frac{s-1}{s} & \frac{1}{s} & \cdots & \frac{1}{s} & 0 \\ \hline & \frac{1}{s} & \frac{1}{s} & \cdots & \frac{1}{s} \end{array}$$

are of the form (31) with $\alpha = \beta = 1/s$. The SSP coefficient for these schemes is $R(\mathbb{A}) = s$. Observe that they are the composition of s explicit Euler steps of length h/s. Observe too that the step-length ratios $d_i = 1/s$, $i = 1, \ldots, s$, agree with the ones in (20) that give the largest SSP coefficient for the composition method.

2. The second order s-stage optimal SSP methods [24, Theorem 9.3]

$$\begin{array}{c|cccc} 0 & 0 & 0 & \cdots & 0 \\ \frac{1}{s-1} & \frac{1}{s-1} & 0 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 1 & \frac{1}{s-1} & \cdots & \frac{1}{s-1} & 0 \\ \hline & \frac{1}{s} & \frac{1}{s} & \cdots & \frac{1}{s} \end{array} \tag{34}$$

are of the form (31) with $\alpha = 1/(s-1)$ and $\beta = 1/s$. For these schemes $R(\mathbb{A}) = s - 1$. However, in this case, although the internal stages are the concatenation of explicit Euler steps of length $h/(s-1)$, these schemes are not composition methods. □

With Lemma 1 and the previous propositions, we can prove the following result.

Proposition 3. *Consider the following Runge-Kutta methods* (A_1, b_1^t), (A_2, b_2^t) *and* (A_3, b_3^t),

$$\begin{array}{c|cccc} 0 & 0 & 0 & \cdots & 0 \\ \gamma & \gamma & 0 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \frac{(n-3)n}{2}\gamma & \gamma & \cdots & \gamma & 0 \\ \hline (A_1, b_1^t) & \gamma & \gamma & \cdots & \gamma \end{array}_{\;\frac{(n-1)(n-2)}{2}} \qquad \begin{array}{c|cccc} 0 & 0 & 0 & \cdots & 0 \\ \alpha & \alpha & 0 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 2(n-1)\alpha & \alpha & \cdots & \alpha & 0 \\ \hline (A_2, b_2^t) & \beta & \beta & \cdots & \beta \end{array}_{\;2n-1} \qquad \begin{array}{c|cccc} 0 & 0 & 0 & \cdots & 0 \\ \delta & \delta & 0 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \frac{(n-2)(n+1)}{n(n-1)}\delta & \delta & \cdots & \delta & 0 \\ \hline (A_3, b_3^t) & \delta & \delta & \cdots & \delta \end{array}_{\;\frac{n(n-1)}{2}} \tag{35}$$

where

$$\gamma = \frac{2}{(n-1)(n-2)}, \qquad \alpha = \frac{1}{n-1}, \qquad \beta = \frac{1}{2n-1}, \qquad \delta = \frac{2}{n(n-1)},$$

and $n \geq 3$. *We denote by* $\mathbb{A}$ *the method obtained from the composition of these schemes with step-length ratios*

$$d_1 = \frac{n-2}{2n}, \qquad d_2 = \frac{1}{n}, \qquad d_3 = \frac{1}{2}. \tag{36}$$

Then, the composition method $\mathbb{A}$ *is an optimal* n^2*-stage third order SSP Runge-Kutta scheme with SSP coefficient* $R(\mathbb{A}) = n^2 - n$.

Proof. First, we compute the order of the composition method. From Lemma 1 we easily obtain the coefficients needed to write down the second order equation (22)

$$-\frac{1}{(n-2)(n-1)}\, d_1^2 + \frac{1}{2}\, d_2^2 - \frac{1}{(n-1)n}\, d_3^2 = 0. \tag{37}$$

Again we use Lemma 1 to compute the coefficients of d_i^3 , $i = 1, \ldots, 3$, in the third order equation (24)

$$\frac{4}{3(n-2)^2(n-1)^2}\, d_1^3 - \frac{1}{3(n-1)}\, d_2^3 + \frac{4}{3(n-1)^2 n^2}\, d_3^3 = 0\,. \tag{38}$$

For $k = 3$, the third order condition (23) is

$$d_1^3(b_1^t c_1^2 - \tfrac{1}{3}) + d_2^3(b_2^t c_2^2 - \tfrac{1}{3}) + d_3^3(b_3^t c_3^2 - \tfrac{1}{3}) + 2d_1 d_2^2(b_2^t c_2 - \tfrac{1}{2}) + 2d_3^2(d_1 + d_2)(b_3^t c_3 - \tfrac{1}{2}) = 0\,.$$

From Lemma 1 we obtain the equation

$$-\frac{3n^2 - 9n + 4}{3(n-2)^2(n-1)^2} d_1^3 + \frac{3n-2}{3(n-1)} d_2^3 - \frac{3n^2 - 3n - 2}{3(n-1)^2 n^2} d_3^3 + d_1 d_2^2 - \frac{2}{(n-1)n} d_3^2(d_1 + d_2) = 0\,. \tag{39}$$

It can be checked that the coefficients d_1, d_2 and d_3 in (36) satisfy equations (37-39) and thus the composition method achieves third order.

Next, we compute the SSP coefficient of the composition method. Schemes (A_1, b_1^t) and (A_3, b_3^t) are the optimal first order SSP methods with $(n-1)(n-2)/2$ and $n(n-1)/2$ stages, respectively. On the other hand, method (A_2, b_2^t) is a $(2n-1)$-stage method of the form (31) with $\alpha = 1/(n-1)$ and $\beta = 1/(2n-1)$, and from Lemma 1, $R(\mathbb{A}_2) = n - 1$. Thus, we get that

$$R(\mathbb{A}_1) = \frac{(n-1)(n-2)}{2}\,, \qquad R(\mathbb{A}_2) = n - 1\,, \qquad R(\mathbb{A}_3) = \frac{n(n-1)}{2}\,. \tag{40}$$

For the composition method with step-length ratios d_i in (36), Proposition 1 gives $R(\mathbb{A}) = n(n-1)$. For $s = n^2$, the third order optimal threshold factor for linear problems is $R(\mathbb{A}) = n(n-1)$ (see [23, Theorem 5.2]) and thus the third order n^2-stage composition method is optimal. □ □

The schemes obtained in the above proposition are the optimal SSP n^2-stage third order method found in [19] in the context of low-storage SSP Runge-Kutta methods. The fact that they are composition of first order schemes gives a new insight in these optimal schemes.

Remark 3. For linear problems, optimal polynomials and optimal threshold factors for s-stage p-th order methods, denoted by $\Phi_{s,p}$ and $R_{s,p}$, respectively have been studied in [23]. In particular, it is proven that for third order n^2-stages, with $n \geq 2$, the threshold factor is $R_{n^2,3} = n(n-1)$ and the stability function is given by

$$\Phi_{n^2,3}(x) = \frac{n}{2n-1}\left(1 + \frac{x}{n(n-1)}\right)^{(n-1)^2} + \frac{n-1}{2n-1}\left(1 + \frac{x}{n(n-1)}\right)^{n^2}$$

This function can be factorized and written as

$$\begin{aligned}\Phi_{n^2,3}(x) &= \left(\frac{n}{2n-1} + \frac{n-1}{2n-1}\left(1 + \frac{x}{n^2-n}\right)^{2n-1}\right)\left(1 + \frac{x}{n(n-1)}\right)^{(n-1)^2} \\ &= \left(1 + \frac{1}{(2n-1)n}\sum_{i=1}^{2n-1} x\left(1 + \frac{x}{n(n-1)}\right)^{i-1}\right)\left(1 + \frac{x}{n(n-1)}\right)^{(n-1)^2} \qquad (41)\end{aligned}$$

where we have used that

$$\left(1 + \frac{x}{r}\right)^m = 1 + \frac{x}{r}\sum_{i=1}^{m}\left(1 + \frac{x}{r}\right)^{i-1}\,.$$

Expression (41) shows that, for linear problems, the optimal method is the composition of several schemes. One of them is a $(2n-1)$-stage method, where the internal stages are the concatenation of explicit Euler steps, and the numerical solution is obtained as a final average of the internal stages. The rest of the schemes in the composition method are one or more methods obtained by composition of explicit Euler steps; all together, the number of explicit Euler steps is $(n-1)^2$. Thus, the factorization of the stability function can be used to show whether a method is a composition method; at the same time, it can also be used to guess the main methods involved in the composition. $\square$

Remark 4.

1. Observe that the SSP coefficient for the composition method is the largest SSP coefficient given in (19), and the step-length ratios d_i in (36) are the values (20) that provide this upper bound.

2. Observe too that scheme (A_3, b_3^t) for $s = n^2$ is the same as scheme (A_1, b_1^t) for $s = (n+1)^2$. $\square$

Next, we display the composition methods in Proposition 3 for the particular cases $n = 3, 4$. We also show the schemes (35) whose composition gives rise to these optimal n^2-stage SSP methods.

Example 5.

1. The composition of schemes

$$
\begin{array}{c|c} 0 & 0 \\ \hline (A_1, b_1^t) & 1 \end{array}
\qquad
\begin{array}{c|ccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{3}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 2 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \\ \hline (A_2, b_2^t) & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \end{array}
\qquad
\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{2}{3} & \frac{1}{3} & \frac{1}{3} & 0 \\ \hline (A_3, b_3^t) & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{array}
$$

with $d_1 = 1/6, d_2 = 1/3, d_3 = 1/2$, gives the optimal 9-stage third-order SSP method with $R(\mathbb{A}) = 6$ and Butcher coefficients

$$
\begin{array}{c|ccccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{3} & \frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{2}{3} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 \\
\frac{5}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{6} & \frac{1}{15} & \frac{1}{15} & \frac{1}{15} & \frac{1}{15} & \frac{1}{15} & 0 & 0 & 0 \\
\frac{2}{3} & \frac{1}{6} & \frac{1}{15} & \frac{1}{15} & \frac{1}{15} & \frac{1}{15} & \frac{1}{15} & \frac{1}{6} & 0 & 0 \\
\frac{5}{6} & \frac{1}{6} & \frac{1}{15} & \frac{1}{15} & \frac{1}{15} & \frac{1}{15} & \frac{1}{15} & \frac{1}{6} & \frac{1}{6} & 0 \\
\hline
(A, b^t) & \underbrace{\frac{1}{6}}_{1} & \multicolumn{5}{c}{\underbrace{\frac{1}{15} \;\; \frac{1}{15} \;\; \frac{1}{15} \;\; \frac{1}{15} \;\; \frac{1}{15}}_{5}} & \multicolumn{3}{c}{\underbrace{\frac{1}{6} \;\; \frac{1}{6} \;\; \frac{1}{6}}_{3}}
\end{array}
$$

2. The composition of schemes

$$\begin{array}{c|ccc}
0 & 0 & 0 & 0\\
\frac{1}{3} & \frac{1}{3} & 0 & 0\\
\frac{2}{3} & \frac{1}{3} & \frac{1}{3} & 0\\
\hline
(A_1, b_1^t) & \frac{1}{3} & \frac{1}{3} & \frac{1}{3}
\end{array}
\qquad
\begin{array}{c|ccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{2}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 & 0 & 0\\
1 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 & 0\\
\frac{4}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0\\
\frac{5}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0\\
2 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0\\
\hline
(A_2, b_2^t) & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7}
\end{array}
\qquad
\begin{array}{c|cccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0 & 0\\
\frac{1}{3} & \frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0\\
\frac{1}{2} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & 0 & 0 & 0\\
\frac{2}{3} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & 0 & 0\\
\frac{5}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & 0\\
\hline
(A_3, b_3^t) & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6}
\end{array}$$

with $d_1 = 1/4$, $d_2 = 1/4$, $d_3 = 1/2$, gives the optimal 16-stage third-order SSP method with $R(\mathbb{A}) = 12$ and Butcher coefficients

$$\begin{array}{c|cccccccccccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{1}{12} & \frac{1}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{1}{6} & \frac{1}{12} & \frac{1}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{1}{4} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{1}{3} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{5}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{1}{2} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{7}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{2}{3} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{3}{4} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{1}{2} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{7}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{12} & 0 & 0 & 0 & 0 & 0\\
\frac{2}{3} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{12} & \frac{1}{12} & 0 & 0 & 0 & 0\\
\frac{3}{4} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & 0 & 0 & 0\\
\frac{5}{6} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & 0 & 0\\
\frac{11}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & 0\\
\hline
(A, b^t) & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{28} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12}\\
 & \multicolumn{3}{c}{\underbrace{\hspace{7em}}_{3}} & \multicolumn{7}{c}{\underbrace{\hspace{18em}}_{7}} & \multicolumn{6}{c}{\underbrace{\hspace{15em}}_{6}}
\end{array}$$

$\square$

6 Conclusions

In this paper we have studied SSP properties of composition Runge-Kutta methods. We have obtained the SSP coefficient of a composition method in terms of the SSP coefficients of the involved schemes and an upper bound of it. These results are valid for both explicit and implicit Runge-Kutta methods. Explicit and implicit SSP composition methods have the well known order barriers $p \leq 4$ and $p \leq 6$, respectively. In this paper we have constructed an 8-stage fourth order SSP explicit composition method to show that the bound $p = 4$ is sharp. Besides, we have also given some examples of explicit and implicit SSP composition methods. In particular, we have shown that the n^2-stage third order optimal SSP methods obtained in [19] are composition of first order SSP methods, obtaining a new insight into these schemes.

Some of the examples given in this paper have also been considered in the context of SSP low-storage methods. In particular, optimal $SSP(s, p)$ schemes in (30), (33) and (34), and optimal $SSP(n^2, 3)$ methods in Proposition 3, have also been studied in the context of explicit SSP low-storage methods with sparse Shu-Osher form (13) [7, 19]. On the other hand, the 4-stage implicit methods in Example 2 are the implicit part of the Implicit-Explicit schemes studied in [2, 25]. If we consider that a low-storage s-stage Runge-Kutta method is one that requires less than the $s+1$ memory registers of a naive implementation, then composition methods are low-storage schemes. However, the set of low-storage methods in the sense of [19] is different from the set of composition schemes. For example, optimal $SSP(s, 2)$ methods in (34) are low-storage schemes [7, p. 84] but they are not composition methods.

This paper provides some results on SSP composition Runge-Kutta methods, nevertheless some interesting issues have not been considered. For example, the construction of a sixth order implicit SSP composition method, to prove whether the order barrier $p = 6$ is sharp; or the study of the largest SSP coefficient for s-stage p-th order SSP composition Runge-Kutta methods, that may be of interest to know to what extent SSP composition methods are competitive compared to other SSP schemes. These will be the topic of a forthcoming research.

7 Proofs of some results in the paper

In this section we prove some of the results of the paper, namely Propositions 1 and 2, and Lemma 1. Some of them will be proven by induction on k, this is the number of methods taking part in the composition. First, we will prove the desired property for $k = 2$, then we will assume that the property holds for the composition of k schemes and finally, we will prove that it also holds for the composition of $k + 1$ methods $\mathbb{A}_i$, $i = 1, \dots, k + 1$, with step-length ratios d_i, $i = 1, \dots, k$, such that $d_1 + \cdots + d_k = 1$. In the induction process we will make use of the assumption below.

Assumption 1. We consider the composition of $k + 1$ schemes as the composition of two methods, namely $\bar{\mathbb{A}}$ and $\mathbb{A}_{k+1}$, with step-length ratios $\bar{d}$ and d_{k+1}, such that $\bar{d} + d_{k+1} = 1$, and $\bar{d} = d_1 + \cdots + d_k$. In addition, method $\bar{\mathbb{A}}$ is the composition of k schemes $\mathbb{A}_i$, $i = 1, \dots, k$, with step-length ratios $d_i/\bar{d}$. Observe that $d_1/\bar{d} + \cdots + d_k/\bar{d} = 1$.

7.1 Proof of Proposition 1

First, we compute the block inequalities (12) for the composition of two schemes. Next, we prove Proposition 1 for $k = 2$, and finally, we prove Proposition 1 by induction on k. We introduce the following notation:

(42)
$$\boldsymbol{A}(r) := (I + rA)^{-1}A\,, \qquad \boldsymbol{e}(r) := (I + rA)^{-1}e\,, \qquad \boldsymbol{b}^t(r) := b^t(I + rA)^{-1}\,, \qquad \phi(r) = 1 - rb^t(I + rA)^{-1}e\,.$$

Lemma 2. *We denote by (A, b^t) the composition of the Runge-Kutta methods (A_1, b_1^t), (A_2, b_2^t) with step* *sizes d_1h, d_2h, where $d_1, d_2 > 0$ and $d_1 + d_2 = 1$. Then,*

(43)

$$(I+rA)^{-1}A = \begin{pmatrix} d_1\,\boldsymbol{A}_1(rd_1) & 0 \\ d_1\,\boldsymbol{e}_2(rd_2)\,\boldsymbol{b}_1^t(rd_1) & d_2\,\boldsymbol{A}_2(rd_2) \end{pmatrix}, \quad (I+rA)^{-1}e = \begin{pmatrix} \boldsymbol{e}_1(rd_1) \\ \phi_1(rd_1)\,\boldsymbol{e}_2(rd_2) \end{pmatrix},$$

(44)

$$b^t(I+rA)^{-1} = \begin{pmatrix} d_1\,\phi_2(rd_2)\,\boldsymbol{b}_1^t(rd_1) \\ d_2\,\boldsymbol{b}_2^t(rd_2) \end{pmatrix}, \qquad 1 - rb^t(I+rA)^{-1}e = \phi_1(rd_1)\,\phi_2(rd_2)\,.$$

Consequently, the SSP coefficient $R(\mathbb{A})$ is the largest r such that $(I+rA)^{-1}$ exists and

(45)

$$\begin{array}{llll} \boldsymbol{A}_1(rd_1) \geq 0 & \boldsymbol{e}_1(rd_1) \geq 0\,, & \boldsymbol{A}_2(rd_2) \geq 0\,, & \boldsymbol{b}_2^t(rd_2) \geq 0\,, \\ \boldsymbol{e}_2(rd_2)\,\boldsymbol{b}_1^t(rd_1) \geq 0\,, & \phi_1(rd_1)\,\boldsymbol{e}_2(rd_2) \geq 0\,, & \phi_2(rd_2)\,\boldsymbol{b}_1^t(rd_1) \geq 0\,, & \phi_1(rd_1)\,\phi_2(rd_2) \geq 0\,. \end{array}$$

Proof. As

$$(I+rA)^{-1} = \begin{pmatrix} (I+rd_1A_1)^{-1} & 0 \\ -rd_1(I+rd_2A_2)^{-1}eb_1^t(I+rd_1A_1)^{-1} & (I+rd_2A_2)^{-1} \end{pmatrix},$$

we get that

$$(I+rA)^{-1}A = \begin{pmatrix} (I+rd_1A_1)^{-1} & 0 \\ -rd_1(I+rd_2A_2)^{-1}eb_1^t(I+rd_1A_1)^{-1} & (I+rd_2A_2)^{-1} \end{pmatrix} \begin{pmatrix} d_1A_1 & 0 \\ d_1eb_1^t & d_2A_2 \end{pmatrix}$$

$$= \begin{pmatrix} d_1\boldsymbol{A}_1(rd_1) & 0 \\ -rd_1^2(I+rd_2A_2)^{-1}eb_1^t(I+rd_1A_1)^{-1}A_1 + d_1(I+rd_2A_2)^{-1}eb_1^t & d_2\boldsymbol{A}_2(rd_2) \end{pmatrix}$$

The (2,1) block can be simplified to

$$-rd_1^2\boldsymbol{e}_2(rd_2)b_1^t(I+rd_1A_1)^{-1}A_1 + d_1\boldsymbol{e}_2(rd_2)b_1^t = d_1\boldsymbol{e}_2(rd_2)b_1^t(I+rd_1A_1)^{-1} = d_1\,\boldsymbol{e}_2(rd_2)\,\boldsymbol{b}_1^t(rd_1)\,,$$

and thus we obtain the first block in (43). In a similar way

$$(I+rA)^{-1}e = \begin{pmatrix} (I+rd_1A_1)^{-1} & 0 \\ -rd_1(I+rd_2A_2)^{-1}eb_1^t(I+rd_1A_1)^{-1} & (I+rd_2A_2)^{-1} \end{pmatrix} \begin{pmatrix} e \\ e \end{pmatrix}$$

$$= \begin{pmatrix} \boldsymbol{e}_1(rd_1) \\ -rd_1(I+rd_2A_2)^{-1}eb_1^t(I+rd_1A_1)^{-1}e + (I+rd_2A_2)^{-1}e \end{pmatrix}.$$

Simplifying the second block we get the second expression in (43)

$$-rd_1\boldsymbol{e}_2(rd_2)b_1^t(I+rd_1A_1)^{-1}e + \boldsymbol{e}_2(rd_2) = \big(1 - rd_1b_1^t(I+rd_1A_1)^{-1}e\big)\,\boldsymbol{e}_2(rd_2) = \phi_1(rd_1)\,\boldsymbol{e}_2(rd_2)\,.$$

Next, we compute

$$b^t(I+rA)^{-1} = \left(d_1 b_1^t, d_2 b_2^t\right) \begin{pmatrix} (I+rd_1A_1)^{-1} & 0 \\ -rd_1(I+rd_2A_2)^{-1}eb_1^t(I+rd_1A_1)^{-1} & (I+rd_2A_2)^{-1} \end{pmatrix}$$

$$= \begin{pmatrix} d_1b_1^t(I+rd_1A_1)^{-1} - rd_1d_2b_2^t(I+rd_2A_2)^{-1}eb_1^t(I+rd_1A_1)^{-1} \\ d_2\boldsymbol{b}_2^t(rd_2) \end{pmatrix}.$$

The first block is reduced to

$$d_1\boldsymbol{b}_1^t(rd_1) - rd_1d_2b_2^t(I+rd_2A_2)^{-1}e\boldsymbol{b}_1^t(rd_1) = d_1\left(1 - rd_2b_2^t(I+rd_2A_2)^{-1}e\right)\boldsymbol{b}_1^t(rd_1) = d_1\,\phi_2(rd_2)\,\boldsymbol{b}_1^t(rd_1)\,,$$

that gives the first expression in (44). Finally, we compute the second part in (44)

$$1 - rb^t(I+rA)^{-1}e = 1 - r\left(d_1b_1^t, d_2b_2^t\right)\begin{pmatrix} \boldsymbol{e}_1(rd_1) \\ \phi_1(rd_1)\,\boldsymbol{e}_2(rd_2) \end{pmatrix} = 1 - rd_1b_1^t\boldsymbol{e}_1(rd_1) - rd_2b_2^t\phi_1(rd_1)\,\boldsymbol{e}_2(rd_2)$$

$$= \phi_1(rd_1) - rd_2b_2^t\phi_1(rd_1)\,\boldsymbol{e}_2(rd_2) = \phi_1(rd_1)(1 - rd_2b_2^t\,\boldsymbol{e}_2(rd_2)) = \phi_1(rd_1)\,\phi_2(rd_2)\,.$$

The result follows from (43-44) and the definition (11) of $R(\mathbb{A})$. □ □

Once we have the block inequalities (12) for the composition of two schemes, we can prove expression (18) in Proposition 1 for $k = 2$.

Lemma 3. *Consider a method $\mathbb{A}$ that is the composition of the SSP schemes $\mathbb{A}_1$ and $\mathbb{A}_2$ with step sizes d_1h, d_2h, where $d_1, d_2 > 0$ and $d_1 + d_2 = 1$. Then, the SSP coefficient $R(\mathbb{A})$ of the composition method is*

$$R(\mathbb{A}) = \min\left\{\frac{R(\mathbb{A}_1)}{d_1}, \frac{R(\mathbb{A}_2)}{d_2}\right\}\,. \tag{46}$$

Proof. Block-wise, the composition method can be written as

$$\begin{aligned} Y_1 &= e \otimes y_n + d_1h(A_1 \otimes I)F(Y_1)\,, \\ y_{n+1}^* &= y_n + d_1h(b_1^t \otimes I)F(Y_1)\,, \\ Y_2 &= e \otimes y_{n+1}^* + d_2h(A_2 \otimes I)F(Y_2)\,, \\ y_{n+1} &= y_n + d_1h(b_1^t \otimes I)F(Y_1) + d_2h(b_2^t \otimes I)F(Y_2)\,. \end{aligned}$$

Thus, if $hd_1 \le R(\mathbb{A}_1)$ and $hd_2 \le R(\mathbb{A}_2)$, we get

$$\|Y_1\| \le \|y_n\|\,, \quad \|y_{n+1}^*\| \le \|y_n\|\,, \quad \|Y_2\| \le \|y_{n+1}^*\| \le \|y_n\|\,, \quad \|y_{n+1}\| \le \|y_{n+1}^*\| \le \|y_n\|\,,$$

and thus,

$$\min\left\{\frac{R(\mathbb{A}_1)}{d_1}, \frac{R(\mathbb{A}_2)}{d_2}\right\} \le R(\mathbb{A})\,.$$

Next, we prove that

$$R(\mathbb{A}) \le \min\left\{\frac{R(\mathbb{A}_1)}{d_1}, \frac{R(\mathbb{A}_2)}{d_2}\right\}\,. \tag{47}$$

For $r = R(\mathbb{A})$, from Lemma 2 we obtain inequalities (45), in particular, $\phi_1(rd_1)\,\phi_2(rd_2) \geq 0$. From the definition of the function ϕ in (42), we can write

$$\phi_1(rd_1)\,\phi_2(rd_2) = \phi_1(rd_1)\left(1 - rd_2 b_2^t \boldsymbol{e}_2(rd_2)\right) = \phi_1(rd_1) - rd_2 b_2^t \phi_1(rd_1)\boldsymbol{e}_2(rd_2) \geq 0\,,$$
$$\phi_1(rd_1)\,\phi_2(rd_2) = \left(1 - rd_1 \boldsymbol{b}_1^t(rd_1)e\right)\,\phi_2(rd_2) = \phi_2(rd_2) - rd_1\phi_2(rd_2)\boldsymbol{b}_1^t(rd_1)e \geq 0\,,$$

that is,

$$\phi_1(rd_1) \geq rd_2 b_2^t \phi_1(rd_1)\boldsymbol{e}_2(rd_2)\,, \qquad \phi_2(rd_2) \geq rd_1\phi_2(rd_2)\boldsymbol{b}_1^t(rd_1)e\,. \tag{48}$$

In (45) we have that $\phi_1(rd_1)\,\boldsymbol{e}_2(rd_2) \geq 0$ and $\phi_2(rd_1)\,\boldsymbol{b}_1^t(rd_1) \geq 0$, and thus, from (48) we obtain that $\phi_1(rd_1) \geq 0$ and $\phi_2(rd_2) \geq 0$. Consequently, $\boldsymbol{e}_2(rd_2) \geq 0$ and $\boldsymbol{b}_1^t(rd_1) \geq 0$. In this way, together with (45), we obtain

$$\begin{aligned} &\boldsymbol{A}_1(rd_1) \geq 0 \quad &&\boldsymbol{e}_1(rd_1) \geq 0\,, \quad &&\boldsymbol{b}_1^t(rd_1) \geq 0\,, \quad &&\phi_1(rd_1) \geq 0\,,\\ &\boldsymbol{A}_2(rd_2) \geq 0\,, \quad &&\boldsymbol{e}_2(rd_2) \geq 0\,, \quad &&\boldsymbol{b}_2^t(rd_2) \geq 0\,, \quad &&\phi_2(rd_2) \geq 0\,. \end{aligned}$$

We have proven that $rd_1 \leq R(\mathbb{A}_1)$, $rd_2 \leq R(\mathbb{A}_2)$ and thus inequality (47) holds. □ □

Proof. of Proposition 1 by induction on k
We use Assumption 1 to consider the composition of $k+1$ schemes as the composition of two methods, namely $\bar{\mathbb{A}}$ and $\mathbb{A}_{k+1}$, with step-length ratios $\bar{d}$ and d_{k+1}, such that $\bar{d} + d_{k+1} = 1$, and $\bar{d} = d_1 + \cdots + d_k$. Besides, $\bar{\mathbb{A}}$ is the composition of the k schemes $\mathbb{A}_i$, $i = 1, \ldots, k$, with step-length ratios $d_i/\bar{d}$. We assume by induction that the SSP coefficient $R(\bar{\mathbb{A}})$ of this composition method is given by (18), that is

$$R(\bar{\mathbb{A}}) = \min\left\{\frac{R(\mathbb{A}_1)}{d_1/\bar{d}}, \ldots, \frac{R(\mathbb{A}_k)}{d_k/\bar{d}}\right\}\,. \tag{49}$$

Now, from Lemma 3 and (49), we trivially obtain

$$R(\mathbb{A}) = \min\left\{\frac{R(\bar{\mathbb{A}})}{\bar{d}}, \frac{R(\mathbb{A}_{k+1})}{d_{k+1}}\right\} = \min\left\{\frac{R(\mathbb{A}_1)}{d_1}, \ldots, \frac{R(\mathbb{A}_k)}{d_k}, \frac{R(\mathbb{A}_{k+1})}{d_{k+1}}\right\}\,. \tag{50}$$

Next, we prove an upper bound for (50). For this purpose, we define the set $\mathcal{I}_{k+1} = \{i \in \{1, \ldots, k+1\} \mid R(\mathbb{A}_i) < \infty\}$. Observe that if $\mathcal{I}_{k+1} = \mathcal{I}_k$ if $R(\mathbb{A}_{k+1}) = \infty$, and $\mathcal{I}_{k+1} = \mathcal{I}_k \cup \{k+1\}$ if $R(\mathbb{A}_{k+1}) < \infty$. Now we can write equation (50) as the minimum of a set of real numbers

$$R(\mathbb{A}) = \min_{i \in \mathcal{I}_{k+1}} \left\{\frac{R(\mathbb{A}_i)}{d_i}\right\}\,. \tag{51}$$

In order to obtain an upper bound for (51), we consider the convex hull of the set or real numbers $\{Z_1, Z_2, \ldots, Z_\ell\}$, where ℓ is the cardinality of $\mathcal{I}_{k+1}$. As the convex hull of the set of real numbers is the line segment joining the outermost two points, we trivially obtain

$$\min\{Z_1, Z_2, \ldots, Z_\ell\} \leq \frac{\alpha_1}{\sum_{i=1}^{\ell}\alpha_i} Z_1 + \cdots + \frac{\alpha_\ell}{\sum_{i=1}^{\ell}\alpha_i} Z_\ell\,, \qquad \text{for all } \alpha_1, \ldots, \alpha_\ell > 0\,. \tag{52}$$

Furthermore, the maximum in (52) is obtained if and only if $Z_i = Z_j$ for all i, j. In that case, the following equality holds

$$Z_i = \frac{\sum_{j=i}^{\ell}\alpha_i Z_i}{\sum_{i=1}^{\ell}\alpha_i}\,. \tag{53}$$

Inequality (52) directly aplied to the set of real numbers in (51) gives us inequality (19). In a similar way, from (53) we obtain the values (20). □ □

7.2 Proof of Proposition 2 (section 4)

The order conditions for linear problems, namely (22) and (24), can be obtained by using Theorem 2 in [17]. Next, we prove the order condition (23) by induction on k, the number of schemes in the composition method. First, we prove this condition for $k = 2$.

Lemma 4. *Consider a method (A, b^t) that is the composition of schemes (A_1, b_1^t) and (A_2, b_2^t) with step-length ratios d_1, d_2, such that $d_1 + d_2 = 1$ and $d_1, d_2 > 0$. Then, the third order condition $b^t c^2 = 1/3$ for the composition method is equivalent to*

$$d_1^3(b_1^t c_1^2 - \tfrac{1}{3}) + d_2^3(b_2^t c_2^2 - \tfrac{1}{3}) + 2d_1 d_2^2(b_2^t c_2 - \tfrac{1}{2}) = 0\,. \tag{54}$$

Proof. A direct computation gives

$$\begin{aligned} b^t c^2 &= (d_1 b_1^t,\ d_2 b_2^t)(d_1^2 c_1^2,\ (d_1 e + d_2 c_2)^2)^t = d_1^3\, b_1^t c_1^2 + d_1^2 d_2\, b_2^t e + 2d_1 d_2^2\, b_2^t c_2 + d_2^3\, b_2^t c_2^2 \\ &= \sum_{i=1}^{2} d_i^3(b_i^t c_i^2 - \tfrac{1}{3}) + 2d_1 d_2^2(b_2^t c_2 - \tfrac{1}{2}) + \tfrac{1}{3}(d_1 + d_2)^3\,. \end{aligned}$$

Now, from the condition $d_1 + d_2 = 1$, we obtain that $b^t c^2 = 1/3$ is equivalent to (54). □ □

Proof of condition (23) *in Proposition 2.* We use Assumption 1 to consider the composition of $k+1$ schemes as the composition of two methods, namely $\mathbb{A}_1$ and $\bar{\mathbb{A}}$, with step-length ratios d_1 and $\bar{d}$, such that $d_1 + \bar{d} = 1$, and $\bar{d} = d_2 + \cdots + d_{k+1}$. In addition, $\bar{\mathbb{A}}$ is the composition of the k schemes $\mathbb{A}_i$, $i = 2, \ldots, k+1$, with step-length ratios $d_i/\bar{d}$. We assume that the third order condition $\bar{b}^t \bar{c}^2 = 1/3$ for the composition method $\bar{\mathbb{A}}$ is equivalent to condition (54), namely

$$\sum_{i=2}^{k+1} \frac{d_i^3}{\bar{d}^3}(b_i^t c_i^2 - \tfrac{1}{3}) + 2\sum_{i=3}^{k+1}\left(\sum_{j=2}^{i-1}\frac{d_j}{\bar{d}}\right)\frac{d_i^2}{\bar{d}^2}(b_i^t c_i - \tfrac{1}{2}) = 0\,. \tag{55}$$

Now we use Lemma 4 for schemes (A_1, b_1^t) and $(\bar{A}, \bar{b}^t)$, and the condition (55) for $(\bar{A}, \bar{b}^t)$ to obtain that

$$\begin{aligned} 0 &= d_1^3(b_1^t c_1^2 - \tfrac{1}{3}) + \bar{d}^3(\bar{b}^t \bar{c}^2 - \tfrac{1}{3}) + 2d_1 \bar{d}^2(\bar{b}^t \bar{c} - \tfrac{1}{2}) \\ &= d_1^3(b_1^t c_1^2 - \tfrac{1}{3}) + \bar{d}^3\left(\sum_{i=2}^{k+1}\frac{d_i^3}{\bar{d}^3}(b_i^t c_i^2 - \tfrac{1}{3}) + 2\sum_{i=3}^{k+1}\left(\sum_{j=2}^{i-1}\frac{d_j}{\bar{d}}\right)\frac{d_i^2}{\bar{d}^2}(b_i^t c_i - \tfrac{1}{2})\right) + 2d_1\bar{d}^2\sum_{i=2}^{k+1}\frac{d_i^2}{\bar{d}^2}(b_i^t c_i - \tfrac{1}{2}) \\ &= \sum_{i=1}^{k+1} d_i^3(b_i^t c_i^2 - \tfrac{1}{3}) + 2\sum_{i=3}^{k+1}\left(\sum_{j=2}^{i-1} d_j\right) d_i^2(b_i^t c_i - \tfrac{1}{2}) + 2d_1\sum_{i=2}^{k+1} d_i^2(b_i^t c_i - \tfrac{1}{2}) \\ &= \sum_{i=1}^{k+1} d_i^3(b_i^t c_i^2 - \tfrac{1}{3}) + 2\sum_{i=3}^{k+1}\left(\sum_{j=1}^{i-1} d_j\right) d_i^2(b_i^t c_i - \tfrac{1}{2}) + 2d_1 d_2^2(b_2^t c_2 - \tfrac{1}{2}) \\ &= \sum_{i=1}^{k+1} d_i^3(b_i^t c_i^2 - \tfrac{1}{3}) + 2\sum_{i=2}^{k+1}\left(\sum_{j=1}^{i-1} d_j\right) d_i^2(b_i^t c_i - \tfrac{1}{2})\,. \end{aligned}$$

7.3 Proof of Lemma 1 (section 5.1)

Part i). Straightforward computations give

$$b^t e = s\,\beta\,, \qquad\qquad b^t c = \alpha\beta \sum_{i=1}^{s-1} i = \frac{1}{2}\alpha\beta(s-1)s\,,$$

$$b^t c^2 = \alpha^2\beta \sum_{i=1}^{s-1} i^2 = \frac{1}{6}\alpha^2\beta(s-1)s(2s-1)\,, \qquad b^t A c = \alpha^2\beta \sum_{i=1}^{s-2} i(s-1-i) = \frac{1}{6}\alpha^2\beta(s-2)(s-1)s\,.$$

Part ii). If we denote $r = 1/\alpha$, we get

$$(I + rA) = \begin{pmatrix} 1 & & & \\ 1 & 1 & & \\ \vdots & \ddots & \ddots & \\ 1 & 1 & \cdots & 1 \end{pmatrix}, \qquad (I + rA)^{-1} = \begin{pmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{pmatrix}.$$

Then

$$(I{+}rA)^{-1}A = \begin{pmatrix} 0 & & & \\ \alpha & 0 & & \\ & \ddots & \ddots & \\ & & \alpha & 0 \end{pmatrix}, \quad (I{+}rA)^{-1}e = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad b^t(I{+}rA)^{-1} = (0,\dots,0,\beta)\,, \quad 1{-}rb^t(I{+}rA)^{-1}e$$

which are nonnegative for $\alpha > \beta > 0$, and, consequently, $R(\mathbb{A}) \geq 1/\alpha$. From (16) we obtain that $R(\mathbb{A}) \leq 1/\alpha$ and thus the result follows. $\square$

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